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Polaronic effects on donor states in III–V and II–VI quantum wells under electric fields

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Abstract. Polaronic effects on the ground state of a donor in $GaAs/Al_{1-x}Ga_xAs$ and $ZnSe/Zn_{1-x}Cd_xSe$ quantum wells under the influence of an external electric field are investigated for the impurity atom doped at various positions. The confined electron interacts with the interface as well as confined phonon modes that exist in such structures. It is found that such effects in II–VI compounds are in general much more significant than in III–V compounds, reflecting the stronger electron–phonon coupling in more ionic II–VI materials. The ground state energy of the impurity is calculated by means of the Lee, Low and Pines transformation. Contributions from confined and interface phonon modes are considered separately and results calculated for various well widths, field strengths and different impurity positions are presented and discussed.

1. Introduction

It was demonstrated more than ten years ago that the electronic properties in a quantum well system change significantly by the application of an external electric field along the growth direction [1]. The polarization induced by the field as well as the energy level shift of the confined carriers are responsible for the intensity decrease and peak shift of the photoluminescence (PL) spectra observed in $GaAs/Al_{1-x}Ga_xAs$ multi-quantum-well structures. Other interesting effects on the PL spectra of p-doped $GaAs/Al_{1-x}Ga_xAs$ samples have also been reported [2]. As a consequence of the energy level change of carriers in the multi-quantum-well system, the optical absorption edge shifts to longer wavelength with increasing field and a new type of high-speed optical modulator is demonstrated in a p–i–n diode structure [3].

On the theoretical side, electric field effects on the energy of confined electrons and holes as well as the overlap integral of electron–hole wave functions are studied by a variational calculation with results relevant to optical processes [4]. The impurity binding energy shift in a quantum well due to the field-induced electronic polarization has also been investigated [5, 6]. Strong dependence on the impurity position is found.

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Although there exist numerous papers on polaron states in quantum wells in magnetic fields [7–14], there have been relatively few works on confined polarons in electric fields. The hydrogenic states of an impurity in quantum wells under an external electric field have been studied in the past [15]. The electric field effect on polaron states in an infinite quantum well has also been investigated [16] by considering the coupling of a confined electron with only bulk longitudinal optical (LO) phonon modes which do not exist in such systems. Moreover, the strong-coupling theory of polarons in quantum well systems has also been discussed [17]. Since the quantum well system can only support confined LO modes and interface modes of lattice vibrations [8, 9], it is therefore necessary in principle to consider these modes in the discussion of polaronic effects in quantum well structures. For wide wells, however, the confinement is rather weak and it is a good approximation to consider only the bulk modes. The properties of polaronic states in a $GaAs/Ga_{1-x}Al_xAs$ double heterostructure under applied magnetic fields have already been studied in great detail by assuming either bulk phonon modes [10] or more realistic confined and interface modes [11–13]. It is well known that the dominant contribution to binding a polaron in a quantum well comes from the Coulomb and confinement potentials, the correction due to electron–phonon interactions is generally small except in the resonant region. When the well width reduces, the bulk modes gradually deviate from realistic modes, especially in external magnetic fields which tend to enhance the interface mode effect [18]. In cases of narrow wells, interface modes can be dominant while the confined modes diminish. In the present paper, we study the binding energy change of a polaron bound to a hydrogenic impurity in both III–V and II–VI compounds due to the applied electric field by means of the Lee–Low–Pines (LLP) transformations. Our purpose is to investigate the electric field influence on contributions from various phonon modes; we are mainly concerned with narrow wells. It is important to remark that strictly speaking there is no bound state in the external electric field, hence our discussion is necessarily limited to field strengths under which the concept of quasi-bound states is valid.

We first outline the theory in section 2, in which we briefly review the electron–phonon interaction Hamiltonian in a quantum well. In section 3 the ground state energy of the polaron is calculated for different impurity positions in the well of $GaAs/Al_{1-x}Ga_xAs$ and $ZnSe/Zn_{1-y}Cd_ySe$ structures as a function of the electric field and the well width. Results of our calculation are presented and discussed in section 4.

2. Theory

Consider a donor impurity atom located at the centre of the quantum well of width d in a $GaAs/Al_{1-x}Ga_xAs$ double-heterostructure (DHS) system. An electric field of strength F is applied along the growth direction. The geometry is illustrated in figure 1. For convenience, we define the two-dimensional (2D) vectors $\boldsymbol{\kappa}$ and $\boldsymbol{\rho}$ such that $\boldsymbol{k} = (\boldsymbol{\kappa}, q)$ and $\boldsymbol{r} = (\boldsymbol{\rho}, z)$ for the phonon momentum and electron position, respectively. The electron momentum is denoted by $\boldsymbol{k}_e = (\boldsymbol{k}, k_z)$. The total Hamiltonian for the system is

$$H = H_e + H_{ph} + H_{e-ph}. \tag{1}$$

The first term in (1) is the Hamiltonian for a hydrogenic impurity confined in the square well at z_i. It is given by

$$H_e = \frac{p^2}{2m} - \frac{e^2}{\varepsilon_1[x^2 + y^2 + (z - z_i)^2]^{1/2}} + V(z) + |e|Fz \tag{2a}$$

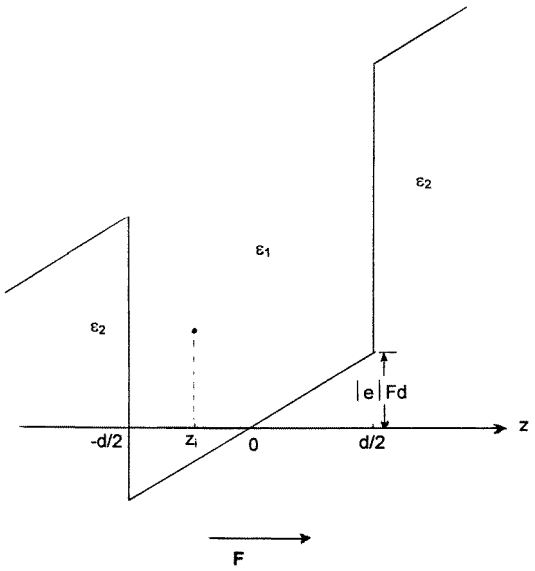

Figure 1. Geometry of the quantum well conduction band. An electric field $\boldsymbol{F}$ is applied in the z-direction.

where we have introduced the confinement potential

$$V(z) = \begin{cases} V_0 & |z| \geqslant d/2 \\ 0 & |z| < d/2. \end{cases} \tag{2b}$$

The electron band mass is denoted by m and d is the well width. The second term represents the free phonon Hamiltonian

$$H_{ph} = H_{LO} + H_{IN} \tag{3a}$$

$$H_{LO} = \sum_{\boldsymbol{\kappa},m} \hbar\omega_{LO}[a_m^\dagger(\boldsymbol{\kappa})a_m(\boldsymbol{\kappa}) + \tfrac{1}{2}] \tag{3b}$$

$$H_{IN} = \sum_{\boldsymbol{\kappa},j} \{\hbar\omega_{sj}[a_{sj}(\boldsymbol{\kappa})a_{sj}(\boldsymbol{\kappa}) + \tfrac{1}{2}] + \hbar\omega_{aj}[a_{aj}(\boldsymbol{\kappa})a_{aj}(\boldsymbol{\kappa}) + \tfrac{1}{2}]\} \tag{3c}$$

where we have defined the creation (annihilation) operators $a_m^\dagger(a_m)$ for the confined modes and $a_{sj,aj}^\dagger(a_{sj,aj})$ for the symmetric and antisymmetric interface phonon modes, respectively. They obey the commutation relations

$$\begin{aligned} &\lfloor a_\alpha^\dagger(\boldsymbol{\kappa}), a_\beta(\boldsymbol{\kappa}')\rfloor = \delta_{\alpha,\beta}\delta(\boldsymbol{\kappa} - \boldsymbol{\kappa}') \\ &[a_\alpha^\dagger(\boldsymbol{\kappa}), a_\beta^\dagger(\boldsymbol{\kappa}')] = [a_\alpha(\boldsymbol{\kappa}), a_\beta(\boldsymbol{\kappa}')] = 0. \end{aligned} \tag{4}$$

The third term in (1) stands for the interaction Hamiltonian [7, 8]. It consists of two terms: the electron interaction with confined LO modes, and the interaction with interface modes. Thus,

$$H_{e-ph} = H_{e-LO} + H_{e-IN} \tag{5a}$$

where the first term

$$H_{e-LO} = -\sum_{\boldsymbol{\kappa}} \mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{\rho}} \left\{ \sum_{m=1,3,\ldots} B_m(\boldsymbol{\kappa}) \cos\left(\frac{m\pi}{d} z\right)[a_m^\dagger(\boldsymbol{\kappa}) + a_m(-\boldsymbol{\kappa})] \right.$$

$$+\sum_{m=2,4,\ldots} B_m(\boldsymbol{\kappa})\sin\left(\frac{m\pi}{d}z\right)[a_m^\dagger(\boldsymbol{\kappa})+a_m(-\boldsymbol{\kappa})]\Bigg\} \qquad |z|<d/2 \tag{5b}$$

$$= -\sum_{\boldsymbol{\kappa},q} B_q(\boldsymbol{\kappa})\,\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{\rho}}\sin q(|z|-d/2)[a_q^\dagger(\boldsymbol{\kappa})+a_q(-\boldsymbol{\kappa})] \qquad |z|\geqslant d/2 \tag{5c}$$

represents the electron interaction with confined LO phonon modes. We note that the phonon wave vector $q=m\pi/d$ is quantized inside the quantum well but continuous in barriers which remain semi-infinite in our model of the DHS. The second term in (5*a*) is

$$H_{e-IN} = -\sum_{\boldsymbol{\kappa},j}\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{\rho}}\Bigg\{B_{sj}(\boldsymbol{\kappa})\frac{\cosh(\kappa z)}{\cosh(\kappa d/2)}[a_{sj}^\dagger(\boldsymbol{\kappa})+a_{sj}(-\boldsymbol{\kappa})]$$

$$-B_{aj}(\boldsymbol{\kappa})\frac{\sinh(\kappa z)}{\sinh(\kappa d/2)}[a_{aj}^\dagger(\boldsymbol{\kappa})+a_{aj}(-\boldsymbol{\kappa})]\Bigg\} \qquad |z|<d/2 \tag{5d}$$

$$= -\sum_{\boldsymbol{\kappa},j}\mathrm{e}^{-\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{\rho}-\kappa(|z|-d/2)}\{B_{sj}(\kappa)[a_{sj}^\dagger(\boldsymbol{\kappa})+a_{sj}(-\boldsymbol{\kappa})]$$

$$-\mathrm{sgn}(z)B_{aj}(\boldsymbol{\kappa})[a_{aj}^\dagger(\boldsymbol{\kappa})+a_{aj}(-\boldsymbol{\kappa})]\} \qquad |z|\geqslant d/2 \tag{5e}$$

represents the electron interaction with interface phonon modes where $\mathrm{sgn}(z)$ is 1 (-1) for positive (negative) z. The normalization constants are given by

$$|B_m(\kappa)|^2 = \frac{1}{Ad}\frac{4\pi e^2\hbar\omega_{L1}}{\kappa^2+(m\pi/d)^2}\left(\frac{1}{\varepsilon_{\infty 1}}-\frac{1}{\varepsilon_{01}}\right) \tag{6a}$$

$$|B_q(\boldsymbol{\kappa})|^2 = \frac{1}{AD}\frac{4\pi e^2\hbar\omega_{L2}}{\kappa^2+q^2}\left(\frac{1}{\varepsilon_{\infty 2}}-\frac{1}{\varepsilon_{02}}\right) \tag{6b}$$

$$|B_{sj}(\kappa)|^2 = \frac{\pi e^2}{A\kappa}\frac{\hbar\omega_{sj}(\boldsymbol{\kappa})}{\bar{\varepsilon}_1\tanh(\kappa d/2)+\bar{\varepsilon}_2} \tag{6c}$$

$$|B_{aj}(\kappa)|^2 = \frac{\pi e^2}{A\kappa}\frac{\hbar\omega_{aj}(\boldsymbol{\kappa})}{\bar{\varepsilon}_1\coth(\kappa d/2)+\bar{\varepsilon}_2}. \tag{6d}$$

The constants A stands for the interface area and D the barrier thickness, $\varepsilon_{\infty\nu}$ and $\varepsilon_{0\nu}$ denote the optic and dielectric constants of material ν, and $\bar{\varepsilon}_\nu(\omega)$ is defined by

$$\frac{1}{\bar{\varepsilon}_\nu} = \frac{1}{\varepsilon_\nu(\omega)-\varepsilon_{0\nu}} - \frac{1}{\varepsilon_\nu(\omega)-\varepsilon_{\infty\nu}} \tag{7}$$

with the dielectric function of material ν given by

$$\varepsilon_\nu(\omega) = \varepsilon_{\infty\nu}(\omega_{L\nu}^2-\omega^2)/(\omega_{T\nu}^2-\omega^2) \tag{8}$$

where we have introduced the index ν to label the material, with $\nu=1$ for the well and $\nu=2$ for the barrier.

On the LLP transformation scheme, the trial wave function is chosen to be

$$|\psi\rangle = \phi(\boldsymbol{r})U|0\rangle \tag{9}$$

where we have defined the phonon vacuum $|0\rangle$. U is a unitary displacement transformation

$$U = \exp\left\{\sum_{\boldsymbol{k},j}[f_j(\boldsymbol{k})a_j^\dagger(\boldsymbol{k})-f_j^*(\boldsymbol{k})a_j(-\boldsymbol{k})]\right\} \tag{10}$$

in which $f_j(\boldsymbol{k})$ is a variational function to be determined by minimizing the energy expectation value of the interacting system. The wave function $\phi(\boldsymbol{r})$ describes the electron ground state and is given by

$$\phi(\boldsymbol{r}) = \sqrt{\frac{2}{\pi\lambda}}\,\mathrm{e}^{-\rho/\lambda}\varphi(z) \tag{11a}$$

with

$$\varphi(z) = \begin{cases} N\cos(k_z z)\exp\left[-\beta\left(\dfrac{z}{d}+\dfrac{1}{2}\right)\right] & |z| < d/2 \\ N\cos(k_z d/2)\exp\left[-\beta\left(\dfrac{z}{d}+\dfrac{1}{2}\right) - k_z'\left(z-\dfrac{d}{2}\right)\right] & |z| \geqslant d/2 \end{cases} \tag{11b}$$

where we have made use of the variational function $\exp[-\beta(z+d/2)]$ introduced in [1] with the variational parameters λ and β. The wave vectors are related to each other by $k_z' = k_z\tan(k_z d/2)$ and are given by the electronic subband energies $k_z = \sqrt{2mE_0/\hbar^2}$ and $k_z' = \sqrt{2m(V_0-E_0)/\hbar^2}$ in which we have defined $E_l = V_0\cos^2((\alpha/2)\sqrt{2mE_l/\hbar^2})$ for $l = 0, 1, 2, \ldots$. The normalization N in (11*b*) is determined by the boundary conditions

$$\left.\frac{\varphi'}{\varphi}\right|_{\pm d/2}(\nu=1) = \left.\frac{\varphi'}{\varphi}\right|_{\pm d/2}(\nu=2) \tag{12}$$

which yields

$$1 = N^2\,\mathrm{e}^{-\beta}\left\{\frac{d}{2\beta}\sinh\beta + \frac{\cos^2(k_z d/2)(k_z'\cosh\beta + (\beta/d)\sinh\beta/d)}{(k_z')^2-(\beta/d)^2} + \frac{(\beta/d)\sinh\beta\cos(k_z d) + k_z\cosh\beta\sin(k_z d)}{2[k_z^2+(\beta/d)^2]}\right\}. \tag{13}$$

3. The ground state of the impurity

With the Hamiltonian and trial wave function given above, we can proceed to calculate the total energy E of the system. Thus, we have

$$E = E_e + E_{ph} + E_{e-LO} + E_{e-IN} = E_e + E_p. \tag{14}$$

The first term refers to the donor ground state energy without phonon interactions. It is given by

$$E_e = \langle\psi|H_e|\psi\rangle = \frac{\hbar^2}{2m\lambda^2} + \frac{\hbar^2}{2m}K_z^2 - \frac{e^2}{\varepsilon_1}f_1(\lambda,\beta) + |e|Ff_2(\beta) \tag{15a}$$

in which we have defined K_z as the z-component of the electron wave vector in the presence of the electric field. It is related to k_z in the absence of external fields by the following relation.

$$K_z^2 = \left(k_z^2 - \frac{\beta^2}{d^2}\right) + N^2\frac{\beta}{d}\,\mathrm{e}^{-\beta}\left\{k_z'\cos^2\left(\frac{k_z d}{2}\right)\left[\frac{\mathrm{e}^{\beta}}{k_z'-\beta/d} - \frac{\mathrm{e}^{-\beta}}{k_z'+\beta/d}\right] - \frac{k_z}{k_z^2+(\beta/d)^2}\left[k_z\sinh\beta\cos(k_z d) - \frac{\beta}{d}\cosh\beta\sinh(k_z d)\right]\right\}. \tag{15b}$$

The other two functions in (15*a*) are defined as

$$f_1(\lambda,\beta) = \int_0^\infty \mathrm{d}Q\left[1+\left(\frac{\lambda Q}{2}\right)^2\right]^{-3/2}\int_{-\infty}^{\infty}\mathrm{d}z\,\varphi^2(z)\exp(-Q|z-z_i|) \tag{15c}$$

$$f_2(\beta) = \int_{-\infty}^{\infty} z\,\mathrm{d}z\,\varphi^2(z) \tag{15d}$$

where Q is just an integration variable. The energy of the phonon system is

$$E_{ph} = \sum_{\boldsymbol{k},\sigma}\hbar\omega_\sigma[|f_\sigma(\boldsymbol{\kappa})|^2 + \tfrac{1}{2}]. \tag{16}$$

The electron–phonon interaction energy has two parts, the contribution from confined phonon modes

$$E_{e-LO} = -\sum_{\boldsymbol{k}}[1+(k\lambda/2)^2]^{-3/2}\Bigg\{\sum_{m=1,3,\ldots} B_m(\kappa)I_{2n+1}[f_m(\boldsymbol{\kappa})+f_m^*(\boldsymbol{\kappa})] + \sum_{m=2,4,\ldots} B_m(\kappa)I_{2n}[f_m(\boldsymbol{\kappa})+f_m^*(\boldsymbol{\kappa})]\sum_{q>0} B_q(\kappa)I_q[f_q(\boldsymbol{\kappa})+f_q^*(\boldsymbol{\kappa})]\Bigg\} \tag{17a}$$

and the contribution from interface modes

$$E_{e-IN} = -\sum_{\boldsymbol{k},j}\left[1+\left(\frac{\kappa\lambda}{2}\right)^2\right]^{-3/2}\{B_{sj}(\kappa)(I_{s1}+I_{s2})[f_{sj}(\boldsymbol{\kappa})+f_{sj}^*(\boldsymbol{\kappa})] - B_{aj}(\kappa)(I_{a1}+I_{a2})[f_{aj}(\boldsymbol{\kappa})+f_{aj}^*(\boldsymbol{\kappa})]\}. \tag{17b}$$

There are a number of matrix elements involved in (17) defined as follows

$$I_{2n} = \langle\varphi(z)|\sin(m\pi z/d)|\varphi(z)\rangle \qquad |z|<d/2 \qquad n=1,2,3,\ldots \tag{18a}$$

$$I_{2n+1} = \langle\varphi(z)|\cos(m\pi z/d)|\varphi(z)\rangle \qquad |z|<d/2 \qquad n=1,2,3,\ldots \tag{18b}$$

$$I_q = \langle\varphi(z)|\sin(q|z|-qd/2)|\varphi(z)\rangle \tag{18c}$$

$$I_{s1} = \langle\varphi(z)|\frac{\cosh(\kappa z)}{\cosh(\kappa d/2)}|\varphi(z)\rangle \qquad |z|<d/2 \tag{18d}$$

$$I_{s2} = \langle\varphi(z)|\exp[-\kappa(|z|-d/2)]|\varphi(z)\rangle \qquad |z|>d/2 \tag{18e}$$

$$I_{a1} = \langle\varphi(z)|\frac{\sinh(\kappa z)}{\sinh(\kappa d/2)}|\varphi(z)\rangle \qquad |z|<d/2 \tag{18f}$$

$$I_{a2} = \langle\varphi(z)|\mathrm{sgn}(z)\exp[-\kappa(|z|-d/2)]|\varphi(z)\rangle \qquad |z|>d/2. \tag{18g}$$

The phonon-related part of the energy is denoted by E_p in (14) only for simplicity.

The variational functions $f_\sigma(\boldsymbol{\kappa})$ where the subscript σ labels the phonon modes, and parameters λ and β, are determined by minimizing the ground state energy (14) according to

$$\frac{\partial E}{\partial f_\sigma} = 0 \tag{19a}$$

$$\frac{\partial E}{\partial \lambda} = 0 \tag{19b}$$

$$\frac{\partial E}{\partial \beta} = 0. \tag{19c}$$

Equation (19*a*) yields

$$f_\sigma = f_\sigma^* = \frac{B_\sigma L_\sigma}{\overline{h}\omega_\sigma[1+(\kappa\lambda/2)^2]^{3/2}}. \tag{20}$$

With the functions f_σ determined in (19), we can rewrite the phonon-related energy as

$$\begin{aligned} E_p &= -\sum_{\boldsymbol{k}}\left[1+\left(\frac{\kappa\lambda}{2}\right)^2\right]^{-3}\Bigg\{\sum_{n=1}^{\infty}\frac{(B_{2n}^2I_{2n}^2+B_{2n+1}^2I_{2n+1}^2)}{\overline{h}\omega_{L1}} + \sum_{q>0}\frac{B_q^2I_q^2}{\overline{h}\omega_{L2}} + \sum_{j=1,2}\left(\frac{B_{sj}^2I_{sj}^2}{\overline{h}\omega_{sj}}+\frac{B_{aj}^2I_{aj}^2}{\overline{h}\omega_{aj}}\right)\Bigg\} \\ &= -[\alpha_1\overline{h}\omega_{L1}f_3(\lambda,\beta)+\alpha_2\overline{h}\omega_{L2}f_4(\lambda,\beta)+\alpha_{s1}\overline{h}f_5(\lambda,\beta)+\alpha_{s2}\overline{h}f_7(\lambda,\beta) \\ &\quad +\alpha_{a1}\overline{h}f_6(\lambda,\beta)+\alpha_{a2}\overline{h}f_8(\lambda,\beta)] \end{aligned} \tag{21}$$

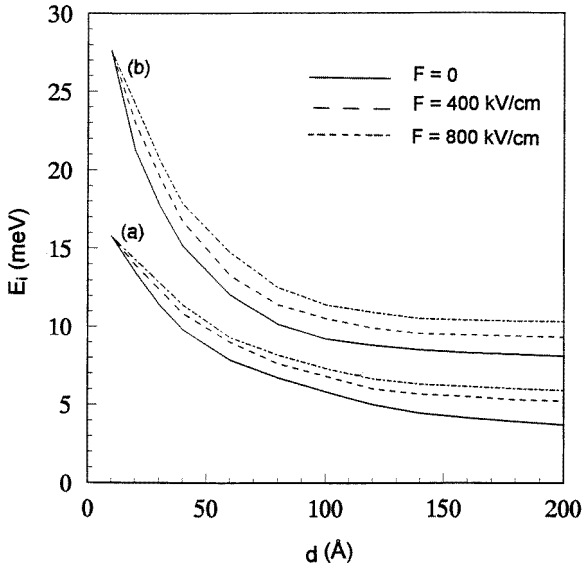

Figure 2. Ionization energy as a function of the well width for the impurity at $z_i = -d/2$ in the quantum well of (a) GaAs/GaAlAs and (b) ZnSe/ZnCdSe structures under various electric fields.

where we have defined the coupling constants

$$\alpha_\nu = \left(\frac{2m\omega_{L\nu}}{\hbar}\right)^{1/2} \frac{e^2}{2\hbar\omega_{L\nu}} \left(\frac{1}{\varepsilon_{\infty\nu}} - \frac{1}{\varepsilon_{0\nu}}\right) \tag{22a}$$

for interactions involving confined phonon modes and the coupling functions

$$\alpha_{sj} = \left(\frac{2n\omega_{sj}}{\hbar}\right)^{1/2} \frac{e^2}{2\hbar\omega_{sj}} \frac{1}{\bar{\varepsilon}_1 \tanh(\kappa d/2) + \bar{\varepsilon}_2} \tag{22b}$$

for interactions involving symmetric interface modes. For antisymmetric interface modes the coupling function is obtained from (22*b*) by simply replacing $\tanh(\kappa d/2)$ by $\coth(\kappa d/2)$ and ω_{sj} by ω_{aj}. Furthermore, we give the explicit form of various functions in (21) as follows.

$$f_3(\lambda, \beta) = \frac{2}{d}\left(\frac{2\hbar}{m\omega_{L1}}\right)^{1/2} \sum_{n=1}^{\infty} \left\{ I_{2n}^2 \int_0^\infty \frac{\kappa \, \mathrm{d}\kappa}{[\kappa^2 + (2n\pi/d)^2][1 + (\kappa\lambda/2)^2]^3} + I_{2n+1}^2 \int_0^\infty \frac{\kappa \, \mathrm{d}\kappa}{\{\kappa^2 + [(2n+1)\pi/d]^2\}[1 + (\kappa\lambda/2)^2]^3} \right\} \tag{23a}$$

$$f_4(\lambda, \beta) = \frac{1}{\pi}\left(\frac{2\hbar}{m\omega_{L2}}\right)^{1/2} \int_0^\infty \frac{\kappa \, \mathrm{d}\kappa}{[1 + (\kappa\lambda/2)^2]^3} \int_0^\infty \frac{I_q^2 \, \mathrm{d}q}{\kappa^2 + q^2} \tag{23b}$$

$$f_{5,7}(\lambda, \beta) = \left(\frac{\hbar}{2m}\right)^{1/2} \int_0^\infty \mathrm{d}\kappa \frac{\sqrt{\omega_{s\nu}(\kappa)}(I_{s1}^2 + I_{s2}^2)}{[1 + (\kappa\lambda/2)^2]^3} \tag{23c}$$

in which $\nu = 1, 2$ for f_5 and f_7 respectively and

$$f_{6,8}(\lambda, \beta) = \left(\frac{\hbar}{2m}\right)^{1/2} \int_0^\infty \mathrm{d}\kappa \frac{\sqrt{\omega_{a\nu}(\kappa)}[I_{a1}^2 + I_{a2}^2]}{[1 + (\kappa\lambda/2)^2]^3} \tag{23d}$$

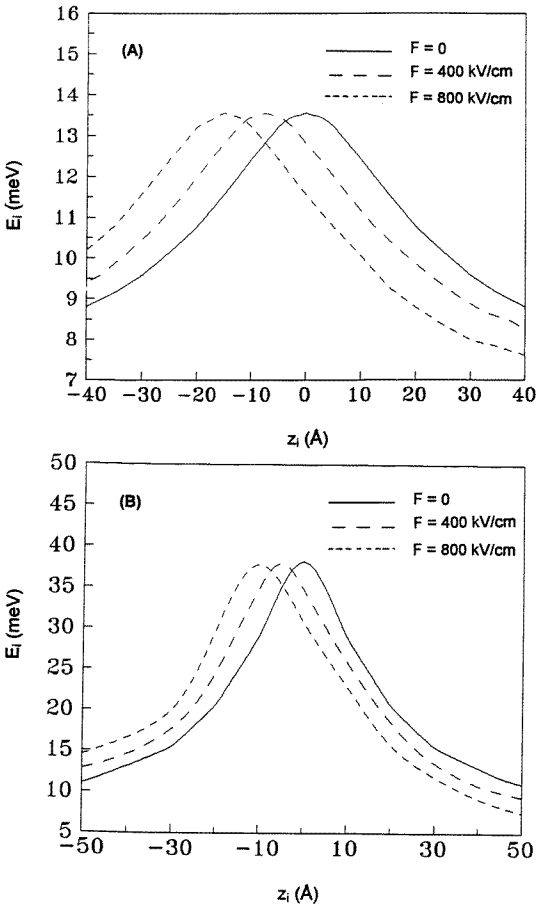

Figure 3. Binding energy of the bound polaron versus the impurity position z_i in a well of width (A) $d = 80$ Å in GaAs/GaAlAs and (B) $d = 100$ Å in ZnSe/ZnCdSe for various electric fields.

in which $\nu = 1, 2$ for f_6 and f_8 respectively. Thus the ground state energy of the donor takes the form

$$E(\lambda, \beta) = \frac{\hbar^2}{2m\lambda^2} + \frac{\hbar^2 K_z^2}{2m} - \frac{e^2}{\varepsilon_1} f_1(\lambda, \beta) + |e|Ff_2(\beta) + E_p(\lambda, \beta). \tag{24}$$

Inserting this in the coupled variational equations (19b, c) and following the standard procedure, we can determine the parameters. However, the calculation can only be carried out on a computer.

As we are concerned with the quasibound state of the polaron by the donor impurity in the well, it is sometimes more convenient to deal with the binding energy. We note that both the confinement energy and the electric field energy are of the order of 1 eV while the Coulomb energy is of order of 1 meV. Hence the electron energy corresponding to its motion in the z-direction is essentially determined by [5]

$$H(z) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_0|e|Fz \tag{25a}$$

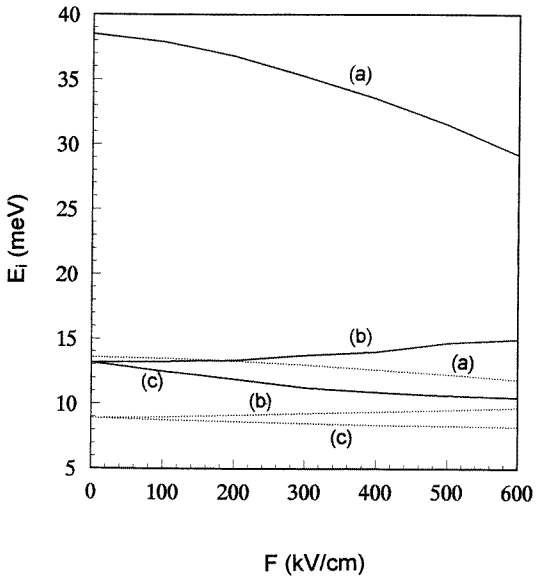

Figure 4. Binding energy of the impurity atom in a quantum well of width $d = 80$ Å in a quantum well of GaAs/GaAlAs (dotted lines) and ZnSe/ZnCdSe (solid lines) versus the applied electric field. The impurity centre is at (a) $z_i = 0$, (b) $z_i = -d/2$ and (c) $z_i = +d/2$.

which implies that

$$E(z) = \frac{\hbar^2 K_z^2}{2m} + |e|Ff_2(\beta). \tag{25b}$$

The binding energy for the impurity centred at z_i is then expressed approximately as

$$E_i = E(z) - \langle H \rangle = E(z) - E(\lambda_0, \beta_0) = \frac{e^2}{\varepsilon_1} f_1(\lambda_0, \beta_0) - \frac{\hbar^2}{2m\lambda_0^2} - E_p(\lambda_0, \beta_0) \tag{26}$$

where λ_0 and β_0 are solutions to the coupled variational equations (19b, c).

4. Results and discussion

We are now ready to calculate the polaron binding energy under various conditions. In our numerical computation, we take $x = y = 0.3$ and other parameters employed are listed in table 1. We first calculate the binding energy or ionization energy of the impurity in (a) a GaAs/$Ga_{0.7}Al_{0.3}$As well and (b) a ZnSe/$Zn_{0.7}Cd_{0.3}$Se well without electron–phonon interactions for different field strengths. Our calculation shows that the electric field influence depends very much on the impurity position in the well. For easier comparison, we present in figure 2 the ionization energy as a function of the well width for an impurity situated at $z_i = -d/2$. It is clearly seen that the binding in the ZnSe well is stronger than that in the GaAs well by almost a factor of 2. The electric field effect tends to increase with increasing well widths. In the absence of external electric fields, our results for the GaAs well can be compared with existing results in the literature [5, 19]. As expected, they agree with those in [5] for $F = 0$, in [19] for $\gamma = 0$.

In figure 3, we plot the binding energy as a function of the impurity position in (A) GaAs/$Ga_{0.7}Al_{0.3}$As and (B) ZnSe/$Zn_{0.7}Cd_{0.3}$Se quantum wells with and without the applied

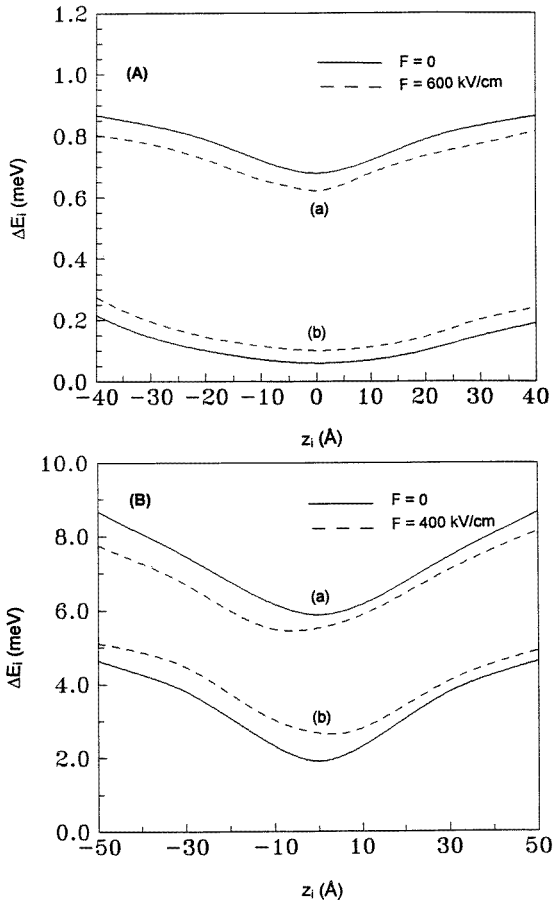

Figure 5. Binding energy correction due to polaronic effects from (a) confined modes and (b) interface modes as a function of the impurity position z_i in the quantum well of (A) GaAs/GaAlAs and (B) ZnSe/ZnCdSe structures.

Table 1. Parameters used in the present calculation.

Material	ε_0	ε_∞	$\hbar\omega_{LO}$ (meV)	$\hbar\omega_{TO}$ (meV)	V_0 (eV)	m	α_{LO}
GaAs	12.5	10.06	36.27	33.85	1.3	$0.067m_0$	0.068
AlAs	10.6	8.16	50.05	44.85	1.3	$0.067m_0$	0.12
ZnSe	8.3	5.8	30.5	25.7	0.6	$0.171m_0$	0.432
CdSe	9.5	6.1	26.45	21.2	0.6	$0.171m_0$	0.46

field. In the absence of external fields, our results in (A) are consistent with those in [10] and [11] for zero magnetic fields. The result in (B) for $F = 0$ and $z_i = 0$ is consistent with that of [17]. It is observed that the binding energy peaks at the centre of the well and drops as the impurity centre moves away from the well centre in both cases. Similar studies of polaronic states with only bulk phonon modes are found in [10] under magnetic fields. When the magnetic field is absent or $\gamma = 0$, the minimum energy of donor states

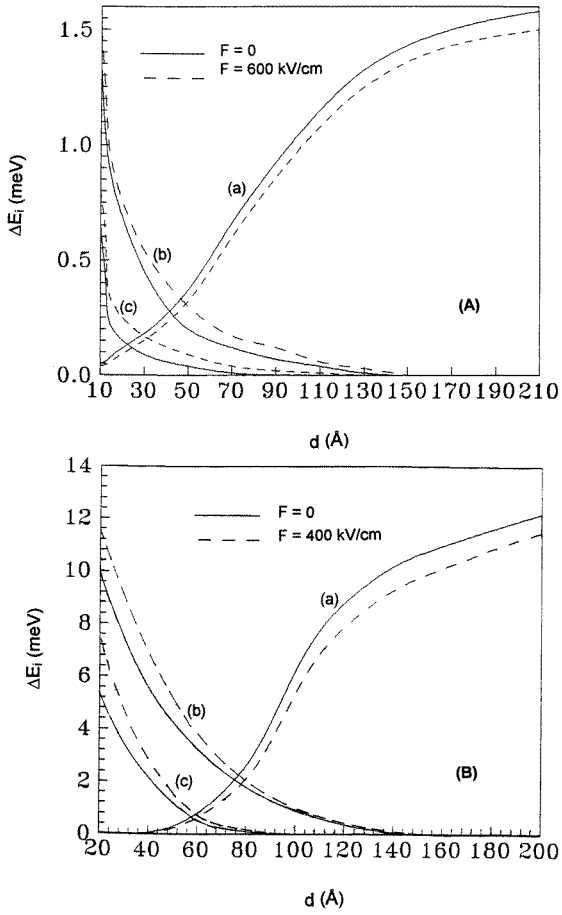

Figure 6. Binding energy correction due to polaronic effects from (a) phonon modes confined in the well, (b) interface modes and (c) modes confined in the barrier as a function of the well width. The impurity centre is at $z_i = -d/4$ in the quantum well of (A) GaAs/GaAlAs and (B) ZnSe/ZnCdSe structures.

occurs at the well centre. This is of course qualitatively consistent with our binding energy results. The maximum binding energy in (B) is larger than in (A) by almost a factor of 3. Even at the interfaces, the binding in (B) is still about 50% stronger than in (A). When the field F is switched on in the growth direction, the peak moves toward the left interface and the displacement increases with increasing fields. These results imply that the electric field tends to suppress the polaron binding energy when the impurity centre is located at $z_i > 0$, and to enhance it when the impurity is at $z_i < 0$. The behaviour is qualitatively similar to previous results for an impurity in infinite wells [16]. On the other hand, it is seen that the peaks in (B) appear much sharper in shape and closer to each other, indicating that the polaron binding is more sensitive to the impurity position but less sensitive to the applied field in (B) than in (A).

The dependence of the polaron binding energy on the electric field is calculated for impurity positions $z_i = 0$ and $\pm d/2$ in both compounds, and the results are plotted in figure 4. The binding in the ZnSe quantum well is once more seen to be much stronger

than in the GaAs well because the former is much more ionic. Since the electric field pulls the electron wave function to the left, it enhances the binding only if $z_i < 0$. In fact, as the figure shows, the binding increases with increasing field for $z_i = -d/2$, but decreases with increasing field for $z_i = 0$ and $+d/2$.

To study the contribution $\Delta E(z_i) = \Delta E_{e-LO} + \Delta E_{e-IN}$ from various phonon modes to the binding energy, we compute the energy correction due to confined and interface modes separately. The results are shown as a function of the impurity position in figure 5 for a GaAs well of width 80 Å in (A) and for a ZnSe well of width 100 Å in (B). We first note by a comparison with figure 3 that the major source of binding comes from the confinement potential and the Coulomb field, the first two terms of (26). It is observed that in general the confined modes dominate the contribution of the electron–phonon interaction in (A) but they are of the same order of magnitude in (B). In both cases, the electron–phonon interaction provides minimum binding corrections when the impurity is at the well centre. The contribution from interface modes is almost doubled in both cases when the impurity centre moves from the centre to the interfaces. What is more interesting is that the electric field enhances the interface mode contribution but reduces the confined mode contribution to the binding. We find further that the field influence is more or less independent of the impurity position in (A) but is apparently more important when the impurity is in the left half of the well in (B).

Contributions from various phonon modes to the polaron self-energy are also calculated as a function of the well width d. The results are presented in figure 6 for $z_i = -d/4$ in (A) the GaAs well and (B) the ZnSe well. It is noted that the contributions from interface and barrier modes may appear somewhat larger than what can be found in the literature where the impurity is usually assumed to be at the well centre. As is expected, the polaron binding is found to be mainly due to the confined modes for large well width. Relatively speaking, the interface modes are more important in (B) than in (A) for the same width. The contribution from modes confined in the barrier is negligible all the time except for very narrow wells. The corrections due to the field are shown by the dashed lines. When $F = 0$, the present results of (A) agree with those given in [11] after the adjustment of the impurity position. Thus, in contrast to the magnetic field which greatly enhances the effect of interface phonon contribution while it suppresses the confined phonon interaction [18], the influence of electric fields is more moderate in general. On the other hand, there exist external electric fields in most cases of practical device applications but external magnetic field is applied mainly for studies of fundamental interest.

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